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13. ABSTRACT *(Maximum 200 words)*

This report summarizes our research on the continuum mechanical modeling of materials that undergo stress- and temperature-induced phase transitions. It contains a problem statement, a summary of results, a list of publications, and names of personnel. The results pertain to the construction of the model, the study of the model in both quasi-static and inertial settings, a study of coupled thermomechanical effects, a study of cyclic effects and comparison with experiments.

14. SUBJECT TERMS
continuum model; phase transformation; shape-memory alloys; thermo-mechanical coupling, cyclic.

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Continuum mechanical modeling of solids undergoing a phase transformation

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TABLE OF CONTENTS

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A. STATEMENT OF PROBLEM STUDIED:

The mechanical properties of a solid are altered if the material undergoes a phase transition, i.e. a change in crystal structure. Thus, under suitable conditions, it may be possible to utilize a phase change in order to improve the properties of a given material.

Many solids, such as plain carbon steels, change phase when they are sufficiently cooled or heated. Certain other solids, such as some Ni-Ti and Cu-Al-Ni alloys, change phase when they are stressed (as well as when the temperature is changed). It is this latter class of materials that were of interest in this research: materials that undergo a phase change under both thermal and mechanical loads.

The principal aim of the research was to develop, and study, a continuum mechanical theory that describes the macroscopic behavior of such materials; particular attention was to be paid to coupled thermo-mechanical effects.

B. SUMMARY OF THE MOST IMPORTANT RESULTS

B1. BRIEF DESCRIPTION

A continuum model for a material that undergoes a thermomechanical phase transformation consists of three ingredients: (i) a Helmholtz free-energy function with multiple energy-wells, (where each energy-well corresponds to a particular phase of the material,) (ii) a nucleation criterion which signals the conditions under which the transformation commences, (at which time material particles begin to move from one energy-well to another,) and (iii) a kinetic relation which specifies the rate at which the transformation progresses (after it has started).

Typically, a material is available in an austenite phase (which is the energetically favorable phase at high-temperatures), and a martensite phase (which is favored at low-temperatures). Martensite exists in many different forms or "variants". When focusing on the uniaxial deformation of a bar, two variants of martensite become particularly relevant: the one in which the longest crystallographic lattice dimension is aligned with the axis of the bar, and the one with the shortest crystallographic dimension aligned with the axial direction of the bar. The former martensite variant (called M^+) is the energetically preferred one when the loading is tensile, the latter (M^-) is preferred under compressive stress.

Our constitutive model was developed, and is described, in [4, 5, 12]. (Throughout this report, papers are referred to by the numbers assigned to them in the publication list in Section C below.) The first ingredient of this model is a three-well Helmholtz free-energy function, the wells corresponding to austenite (called A) and the two variants of martensite M^+ and M^-. The analytical formula defining each energy-well is quadratic in strain but is more complicated in temperature; see [5, 12]. It is chosen such that A, M^+ and M^- each have a constant elastic modulus, coefficient of thermal expansion and specific heat. Moreover, as the temperature is raised, the A energy-well is lowered relative to the M^+ and M^- wells, thus making A the high temperature phase. In the Helmholtz free- energy, the M^+ and M^- wells are always at the same height, which ensures that these are two variants

of each other. On the other hand, the corresponding energy-wells in the potential energy function do not necessarily have the same height; the M^+ well is lower for tensile stress and the M^- well is lower for compressive stress.

We have studied two types of kinetic relations (the second ingredient in our model). The first of these (considered in [4, 5]) is based on the physical mechanism of thermal activation. Here, the idea is that particles in one phase (at the atomistic level) do not all have the same energy but rather that there is a certain probabilistic energy distribution. Thus, some particles have more energy that others and may have sufficient energy to jump over the energy barrier that separates one energy-well from the next. A calculation based on this idea leads to a particular expression for the kinetic relation -- the "thermally activated kinetic relation"-- and relates (in a particular manner) the velocity of a phase boundary to the driving force and temperature. The second kinetic relation that we studied (in [12]) is not based on any micromechanical mechanism but rather on direct macroscopic experiments. This kinetic relation gives two constant vales of driving force, one for the forward transformation and one for the reverse transformation; no transformation takes place for values of driving force between these two values.

For the final ingredient of our theory, the nucleation criterion, we studied the experimentally based model which says that the transformation is initiated when the driving force reaches a critical value. A careful study of the experimental literature indicated that this is the case only at sufficiently slow loading rates. At fast loading rates, multiple nuclei of the second phase are nucleated, and the nucleation criterion should both predict the stress-temperature conditions at which the transformation nucleates, as well as determine the number of nuclei. The most general nucleation criterion that we studied (in [12]) accounts for this too.

After constructing our model, we used it to study a number of different issues. In [4] we examined the response predicted by a two-well model in isothermal loading at various loading rates, as well as in thermal loading at constant stress at various heating rates. This was generalized to a three-well model in [5]. This more general model is capable of describing a much wider variety of phenomena such as the shape-memory effect. With this model we were also able to successfully characterize in [5] another, quite complicated experiment, in which an oscillatory stress was applied to a bar of shape-memory material and simultaneously, its temperature was raised and then decreased.

We showed in [12] that our model is in good agreement with experiment. We studied the effect of cyclic loading in [12] and modified our Helmholtz free-energy function of [4,5] to account for the effect of incoherency dislocations. This was achieved by introducing an internal variable describing the density of precipitated dislocations. A variety of cyclic experiments were then successfully modeled. We also studied the phenomenon of thermal hardening in [9, 12]. By not assuming the bar to be always at a constant temperature during a tensile test, but rather by accounting for the effect of the local heating which occurs due to the heat released by the transformation, we were able to capture and model this phenomenon. The reason that this phenomenon occurs is essentially that, as the austenite-to-martensite transformation occurs under tensile loading, the heat released raises

the temperature near the transformation front; however, austenite is the preferred phase at high temperatures, and so the austenite-to-martensite transformation becomes harder to continue: this leads to the hardening effect. A related phenomenon that we also studied in [12] is the apparently different response of shape-memory materials depending on the environment: there are experiments which show that the stress-elongation behavior of, say NiTi, is different if the test is carried out in air or in a water bath; we have explained this effect and modeled it successfully. A number of results from the dissertation [12] will be published in refereed journals.

We also studied the role of inertia in rapid transformations, such as the impact loading of a bar. In [2, 6] we considered purely mechanical problems while in [7, 8] we considered the coupled thermo-mechanical problem. In [7] we accounted for the effects of heat transfer along the bar, whereas in [8] we considered an adiabatic theory.

B2. <u>ABSTRACTS OF RELEVANT PAPERS:</u>

[2]. R. Abeyaratne and J.K. Knowles, Reflection and transmission of waves from an interface with a phase-transforming solid, *Journal of Intelligent Material Systems and Structures*, **3**, 1992, pp. 224-244.

This paper is concerned with waves in a composite elastic bar, the left half of which is composed of a linearly elastic material, while the nonlinearly elastic material on the right half can undergo a phase transition. We assume that a wave in the left portion of the bar is incident upon the interface between the two materials, and we investigate the question of whether the phase transition can be exploited to augment or diminish the strength of the reflected or transmitted wave.

[4]. R. Abeyaratne and J.K. Knowles, A continuum model of a thermoelastic solid capable of undergoing phase transitions, *Journal of the Mechanics and Physics of Solids*, **41**, 1993, pp. 541-571.

We construct explicitly a Helmholtz free energy, a kinetic relation and a nucleation criterion for a one-dimensional thermoelastic solid, capable of undergoing either mechanically- or thermally-induced phase transitions. We study the hysteretic macroscopic response predicted by this model in the case of quasi-static processes involving stress cycling at constant temperature, thermal cycling at constant stress, or a combination of mechanical and thermal loading that gives rise to the shape-memory effect. These predictions are compared qualitatively with experimental results.

[5]. R. Abeyaratne, S-J. Kim and J.K. Knowles, A one-dimensional continuum model for shape-memory alloys, *International Journal for Solids and Structures*, **31**, 1994, pp. 2229-2249.

In this paper we construct an explicit one-dimensional constitutive model that is capable of describing some aspects of the thermomechanical response of a shape-memory alloy. The model consists of a Helmholtz free-energy function, a kinetic relation and a nucleation criterion. The free-energy is associated with a three-well potential energy function; the kinetic relation is based on thermal activation theory; nucleation is assumed to

occur at a critical value of the appropriate energy barrier. The predictions of the model in various quasi-static thermomechanical loadings are examined and compared with experimental observations.

[6]. Y. Lin, A Riemann problem for an elastic bar that changes phase, *Quarterly of Applied Mathematics*, accepted for publication, to appear 1994.

This paper is concerned with the dynamics of an elastic bar that can undergo reversible stress-induced phase transformations. We consider a Riemann problem in which the initial strains belong to a single metastable phase and prove uniqueness of solution that satisfy a nucleation criterion and a kinetic law at all subsonic and sonic phase boundaries. This paper generalizes the results of an earlier paper; the authors of that paper considered a piecewise linear material for which no wave fans exist, shock waves always travel at the acoustic speed and shock waves are dissipation-free. The material model of the present paper does not suffer from these degeneracies.

[7]. R. Abeyaratne and J.K. Knowles, Dynamics of propagating phase boundaries: thermoelastic solids with heat conduction, *Archive for Rational Mechanics and Analysis*, accepted for publication, to appear 1994.

This paper is concerned with the incorporation of thermal effects into the continuum modeling of dynamic solid-solid phase transitions. The medium is modeled as a thermoelastic solid characterized by a specific Helmholtz free energy potential and a specific kinetic relation. Heat conduction and inertia are taken into account. An initial value problem that gives rise to both shock waves and a propagating phase boundary is analyzed on the basis of this model.

[8]. R. Abeyaratne and J.K. Knowles, Dynamics of propagating phase boundaries: adiabatic theory for thermoelastic solids, *Physica D*, accepted for publication, to appear 1994.

This paper examines adiabatic processes in a thermoelastic material undergoing a solid-solid phase transition. It is shown that an initial-value problem of Riemann type, based on momentum balance, energy balance, kinematic compatibility and the entropy inequality, has a one parameter family of solutions for a range of given data. Within this adiabatic setting, the notions of driving traction and kinetic relation are discussed. The enforcement of a kinetic relation at phase boundaries is shown to single out a particular solution of this Riemann problem from among the family of available solutions.

[9]. S-J. Kim and R. Abeyaratne, On the effect of the heat generated during a stress-induced thermoelastic phase transformation, *Continuum Mechanics and Thermodynamics*, accepted for publication, to appear 1994.

In this paper we examine the stress-elongation response of a bar undergoing a thermoelastic phase transition. Attention is focused on how this response is affected by the heat generated during the transformation. The analysis is based on a continuum model consisting of a two-well Helmholtz free-energy function, a kinetic relation and a nucleation

criterion. The governing mathematical problem is related to one that describes a moving heat source, except that here, the strength and the speed of the source are not known a priori and the energy field equation involves coupling between thermal and mechanical effects. The heat generated by the transformation is found to have a significant effect on the mechanical response whenever the prescribed elongation-rate is moderately large.

[11]. S. Sounderarajan, Stability of a planar phase boundary endowed with surface structure in anti-plane deformations, SM dissertation.

This work investigates the linear stability of a purely mechanical two-phase transformation process involving a planar phase boundary. The phase boundary is endowed with surface structure using a special case of Gurtin & Struthers theory of dissipative accretion that is valid for purely mechanical anti-plane shear deformations. Using a normal mode analysis, it is shown, in both inertial and inertia-free settings, that interface growth is unstable when the appropriate kinetic relation -- a supplementary constitutive relation between the interfacial driving force and the normal interfacial velocity -- is locally decreasing as a function of the normal interfacial velocity. The inclusion of surface structure is found to have no effect upon the stability of the transformation process, per se, but is seen to affect the decay rate of perturbations in an inertia-free setting and may affect the eventual morphologies of the transforming material in both inertial and inertia-free contexts.

[12]. S-J. Kim, A continuum model for phase transitions in thermoelastic solids and its application to shape memory alloys, PhD dissertation.

This thesis is focused on the construction of an explicit one-dimensional continuum model of solids that undergo stress- and temperature-induced phase transitions, and its application to Ni-Ti shape memory alloys. It can be divided into four parts: *First,* a complete one-dimensional constitutive model is constructed. The Helmholtz free-energy function here has three energy wells associated with austenite and two variants of martensite. The nucleation criterion describes the nucleation of multiple phase boundaries based on some experimental observations; it signals the conditions under which the transition from one phase to another commences based on a critical value of driving force. Two examples of kinetic relations are introduced and used to calculate the thermomechanical response of the model. *Secondly,* the thermomechanical predictions of the model are calculated and qualitatively compared with experiments. A numerical algorithm is developed to solve a moving boundary problem associated with stress-induced transformations by combining a standard finite difference method with a Lagrangian interpolation equation. *Thirdly,* the Helmholtz free-energy is modified to take into account the effect of cyclic loading and unloading on the transformation characteristics of the material. Two internal variables are added to the energy function to describe the changes in the free energy of the martensite phases during phase transformations. It turns out that this model simulates successfully various cyclic effects such as the two-way shape memory effect. *Finally,* the model is used to simulate recent experiments on Ni-Ti shape memory wires. The predictions are in agreement with experimental observations.

C. LIST OF PUBLICATIONS

C1. PAPERS PUBLISHED IN REFEREED JOURNALS:

1*. H.S. Hou and R. Abeyaratne, Cavitation in elastic and elastic-plastic solids, *Journal of the Mechanics and Physics of Solids*, **40**, 1992, pp. 571-592.

2. R. Abeyaratne and J.K. Knowles, Reflection and transmission of waves from an interface with a phase-transforming solid, *Journal of Intelligent Material Systems and Structures*, **3**, 1992, pp. 224-244.

3*. H.S. Hou, A study of combined asymmetric and cavitated bifurcations in neo-hookean material under symmetric dead loading, *ASME Journal of Applied Mechanics*, **60**, 1993, pp. 1-7.

4. R. Abeyaratne and J.K. Knowles, A continuum model of a thermoelastic solid capable of undergoing phase transitions, *Journal of the Mechanics and Physics of Solids*, **41**, 1993, pp. 541-571.

5. R. Abeyaratne, Sang-Joo Kim and J.K. Knowles, A one-dimensional continuum model for shape-memory alloys, *International Journal for Solids and Structures*, **31**, 1994, pp. 2229-2249.

6. Y. Lin, A Riemann problem for an elastic bar that changes phase, *Quarterly of Applied Mathematics*, accepted for publication, to appear 1994.

7. R. Abeyaratne and J.K. Knowles, Dynamics of propagating phase boundaries: thermoelastic solids with heat conduction, *Archive for Rational Mechanics and Analysis*, accepted for publication, to appear 1994.

8. R. Abeyaratne and J.K. Knowles, Dynamics of propagating phase boundaries: adiabatic theory for thermoelastic solids, *Physica D*, accepted for publication, to appear 1994.

9. S-J. Kim and R. Abeyaratne, On the effect of the heat generated during a stress-induced thermoelastic phase transformation, *Continuum Mechanics and Thermodynamics*, accepted for publication, to appear 1994.

C2. THESES:

10*. H.S. Hou, Cavitation instability in solids, PhD.

11. S. Sounderarajan, Stability of a planar phase boundary endowed with surface structure in anti-plane deformations, SM.

12. S-J. Kim, A continuum model for phase transitions in thermoelastic solids and its application to shape memory alloys, PhD.

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* These publications were completed during the time when the present grant was in effect but is based on work carried out under my immediately preceding ARO grant (on cavitation).

C3. ORAL PRESENTATIONS:

a. As Organizer of a Conference Session
1. Session on "Phase Transformations" at the conference Contemporary Developments in Solid Mechanics", California Institute of Technology, March 1991.
2. Session on "Phase Transformations" as part of the Eringen Medalist Symposium, Annual Meeting of the Society of Engineering Science, Gainesville, Florida, November 1991.

b. At Conferences
1. 18th International Congress of Theoretical and Applied Mechanics, Haifa, Israel, August 1992.
2. Workshop on Non-equilibrium Systems, Institute for Theoretical Physics, University of California at Santa Barbara, November 1992.
3. Workshop on Martensite, University of Minnesota, Minneapolis, September 1993.
4. Conference on Microstructures and Phase Transitions in Solids, Euromech, Udine, Italy, May 1994.

c. At University Colloquia
1. Materials Science Seminar, Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, October 1992.
2. Mechanics of Materials seminar, University of Minnesota, Minneapolis, November 1992.
3. Aerospace Engineering and Mechanics seminar, University of Minnesota, Minneapolis, December 1992.
4. Applied Mathematics Seminar, Glasgow University, Scotland, April 1993.
5. Applied Mathematics Seminar, Heriot-Watt University, Scotland, April 1993.
6. Solid Mechanics Seminar, Cambridge University, England, April 1993.
7. Applied Mathematics Seminar, Bath University, England, April 1993.
8. Solid Mechanics seminar, Technical University of Denmark, Denmark, April 1993.
9. Thermodynamics and Continuum Mechanics seminar, Technical University of Berlin, Germany, April 1993.
10. Solid Mechanics seminar, Ecole Polytechnique, Palaiseau, France, April 1993.
11. Solid Mechanics seminar, Shell Research Laboratories, The Netherlands, May 1993.
12. Mechanical Engineering seminar, University of Pennsylvania, October 1993.
13. Solid Mechanics seminar, Brown University, November 1993.
14. Aerospace Engineering seminar, University of Michigan, December 1993.

D. LIST OF ALL PARTICIPATING SCIENTIFIC PERSONNEL:

Rohan Abeyaratne (Associate Professor)
Hang-sheng Hou (Graduate student)
Sang-Joo Kim (Graduate student)

DEGREES AWARDED:

Hang-sheng Hou, PhD, June 1991.
Sang-Joo Kim, PhD, October 1994.
Srinivasan Sounderarajan, SM, September 1992.